

Spectral function and fidelity susceptibility in quantum critical phenomena

Shi-Jian Gu* and Wing Chi Yu

Department of Physics and ITP, The Chinese University of Hong Kong, Hong Kong, China

(Dated: August 12, 2014)

In this paper, we derive a simple equality that relates the spectral function $I(k, \omega)$ and the fidelity susceptibility χ_F , i.e. $\chi_F = \lim_{\eta \rightarrow 0} \frac{\pi}{\eta} I(0, i\eta)$ with η being the half-width of the resonance peak in the spectral function. Since the spectral function can be measured in experiments by the neutron scattering or the angle-resolved photoemission spectroscopy (ARPES) technique, our equality makes the fidelity susceptibility directly measurable in experiments. Physically, our equality reveals also that the resonance peak in the spectral function actually denotes a quantum criticality-like point at which the solid state seemingly undergoes a significant change.

PACS numbers: 05.30.Rt, 75.40.Gb, 64.60.-i, 03.67.-a

At zero temperature, the ground-state properties of a quantum many-body system can change quantitatively as the system's parameter varies across a critical point. Because of the absence of thermal fluctuation, the quantitative change is solely driven by quantum fluctuation and hence is called a quantum phase transition [1]. Examples of quantum phase transitions include Mott-insulator transitions and fractional quantum Hall liquids. In the perspective of the quantum information science [2], the ground-state wavefunctions on both sides of the critical point λ_c have distinct structures and if we compare two ground states separated by a small fixed distance $\delta\lambda$ in the parameter space, i.e. the fidelity $|\langle \psi_0(\lambda) | \psi_0(\lambda + \delta\lambda) \rangle|$, is expected to show a minimum at the critical point λ_c [3, 4]. The quantum phase transition in the perspective of the fidelity have been verified in many strongly correlated systems [5–8]. On the other hand, since the structure of the ground-state wavefunction undergoes a significant change as the system is driven adiabatically across the transition point, we can also imagine that the leading term of the fidelity, i.e. the fidelity susceptibility which denotes the leading response of the ground state to the driving parameter, should be a maximum or even divergent at the transition point [9, 10]. Besides, the fidelity between two ground states separated by a long distance in the parameter space also manifests distinct information about quantum phase transitions [11, 12]. Due to the remarkable properties of the fidelity around the critical point [12–15], the fidelity has become an efficient way to detect the quantum transition point in quantum many-body systems [16–27]. Especially, the fidelity has proven to be able to detect unconventional phase transitions such as the topological phase transition too [17–20].

Despite of the great success of the fidelity approach to quantum phase transitions in theory, little progress has been achieved in experiments. Up to now, the only experimental detection of the quantum phase transition in terms of fidelity is based on a spin dimer system via the technique of the nuclear-magnetic-resonance quan-

tum simulator [28]. For a large quantum many-body system, say having a size $L > 10$, to measure the overlap of its two ground states separated by a short distance in the parameter space seems hard to be realized. The interesting scaling and universality behaviors of the fidelity susceptibility in quantum phase transitions still cannot be verified in experiments. Therefore, it is highly expected to find a way to measure the fidelity and its susceptibility directly or indirectly in experiments.

In this paper, we finally derive a neat equality that connects two seemingly unrelated quantities, i.e. the spectral function and fidelity susceptibility. Since the spectral function can be measured in experiments by such as the neutron scattering or ARPES technique [29], such an equality actually makes the fidelity susceptibility directly measurable in experiments. On the other hand, as the most typical model in quantum phase transitions, the transverse-field Ising model and its quantum criticality now can be studied in experiment via the neutron scattering [30]. A possible experimental scheme to measure the fidelity susceptibility of the transverse-field Ising model is proposed.

To begin with, we consider the propagation properties of a single electron in a solid-state system. Without the loss of generality, we assume that the system can be described by a Hubbard-like model whose Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_j n_{j,\uparrow} n_{j,\downarrow} + H_V, \quad (1)$$

where $\langle \rangle$ denotes the summation over all the nearest neighboring pairs, $c_{j,\sigma}^\dagger (c_{j,\sigma})$ is the creation(annihilation) operator for electrons with spin $\sigma = \uparrow, \downarrow$ at site j , t is the hopping integral, $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$, U is the strength of on-site Coulomb interaction, and H_V denotes other types of interactions. In a solid-state system, the total number of electrons is a good quantum number and is decided by the chemical potential of the system. Let us assume that the sample system has N electrons. In this subspace, the eigenstates of the system are decided by the Schrödinger equation

$$H|\psi_n^N\rangle = E_n|\psi_n^N\rangle. \quad (2)$$

*Electronic address: sjgu@phy.cuhk.edu.hk

At zero temperature, the propagation of a single electron in the ground state $|\psi_0^N\rangle$ can be described by the one-electron Green's function in the momentum-energy space

$$G^\pm(k, \omega) = \sum_m \frac{|\langle \psi_m^{N\pm 1} | c_k^\pm | \psi_0^N \rangle|^2}{\omega + E_0^N - E_m^{N\pm 1} + i\eta}, \quad (3)$$

where $|\psi_m^{N\pm 1}\rangle$ is the eigenstate of the Hamiltonian in the subspace of $N \pm 1$ electrons and $c_k^\pm = c_{k\sigma}^\pm (c_k^- = c_{k\sigma})$,

$$c_{k\sigma}^\dagger = \frac{1}{\sqrt{V}} \sum_j e^{-ij\mathbf{k}} c_{j,\sigma}^\dagger \quad (4)$$

with V being the volume of the system. The one-electron spectral function

$$I^\pm(k, \omega) = -\frac{1}{\pi} \text{Im} G^\pm(k, \omega) \quad (5)$$

defines the one-electron addition and removal spectra. $I^\pm(k, \omega)$ can be probed in the inverse and direct photoemission, respectively [29]. From Eq. (3), we have

$$I^\pm(k, \omega) = \lim_{\eta \rightarrow 0} \sum_m \frac{\eta}{\pi} \frac{|\langle \psi_m^{N\pm 1} | c_k^\pm | \psi_0^N \rangle|^2}{(\omega + E_0^N - E_m^{N\pm 1})^2 + \eta^2}. \quad (6)$$

We notice the right-hand side of Eq. (6) actually denotes the leading response of the ground state in the photoemission process. Precisely, the form of $I^\pm(k, \omega)$ is already the same as the dynamic fidelity susceptibility introduced in Ref. [9]. To observe this, we need to consider the effective Hamiltonian including the subspace of both $N - 1$ and $N + 1$ electrons,

$$H(\eta) = \begin{pmatrix} H(N-1) - \omega & \eta c_k^+ & \\ \eta c_k^- & H(N) & \eta c_k^+ \\ & \eta c_k^- & H(N+1) - \omega \end{pmatrix} \quad (7)$$

where ω is due to the photon absorption and emission and η is the strength of the perturbation. When $\eta = 0$, the initial ground state of the system $|\psi_0^N\rangle$ locates in the subspace of N electrons. Then if a small perturbation $\eta(c_k^+ + c_k^-)$ is turned on, the state becomes, to the first order,

$$|\psi_0(\eta)\rangle = |\psi_0^N\rangle + \eta \sum_m \frac{\langle \psi_m^{N+1} | c_k^+ | \psi_0^N \rangle |\psi_m^{N+1}\rangle}{\omega + E_0^N - E_m^{N+1}} + \eta \sum_m \frac{\langle \psi_m^{N-1} | c_k^- | \psi_0^N \rangle |\psi_m^{N-1}\rangle}{\omega + E_0^N - E_m^{N-1}}. \quad (8)$$

According to the definition [3], the fidelity between $|\psi_0^N\rangle$ and $|\psi_0(\eta)\rangle$ becomes

$$|\langle \psi_0^N | \psi_0(\eta) \rangle| = 1 - \frac{\eta^2}{2} \chi_F + \dots \quad (9)$$

where

$$\chi_F = \sum_m \frac{|\langle \psi_m^{N+1} | c_k^+ | \psi_0^N \rangle|^2}{(\omega + E_0^N - E_m^{N+1})^2} + \sum_m \frac{|\langle \psi_m^{N-1} | c_k^- | \psi_0^N \rangle|^2}{(\omega + E_0^N - E_m^{N-1})^2} \quad (10)$$

is the so-called fidelity susceptibility. In Ref. [9], we introduced the concept of dynamic fidelity susceptibility as

$$\chi_F(\eta) = \sum_m \frac{|\langle \psi_m^{N+1} | c_k^+ | \psi_0^N \rangle|^2}{(\omega + E_0^N - E_m^{N+1})^2 + \eta^2} + \sum_m \frac{|\langle \psi_m^{N-1} | c_k^- | \psi_0^N \rangle|^2}{(\omega + E_0^N - E_m^{N-1})^2 + \eta^2}. \quad (11)$$

Since $I(k, \omega) = I^+(k, \omega) + I^-(k, \omega)$, compare the above equation with Eq. (6), we obtain the following equality

$$I(k, \omega) = \lim_{\eta \rightarrow 0} \frac{\eta}{\pi} \chi_F(\eta), \quad (12)$$

or the inverse

$$\chi_F = \lim_{\eta \rightarrow 0} \frac{\pi}{\eta} I(k, \omega + i\eta), \quad (13)$$

which is the key result of this work.

The equality about the fidelity susceptibility and the spectral function is remarkable. The former is a quantum information theoretic concept used to study quantum phase transitions. Physically, the divergence of the fidelity susceptibility manifests a significant change occurred in the structure of the ground-state wavefunction, hence denotes a phase transition. Lots of attentions have been paid to the fidelity and fidelity susceptibility approach to quantum phase transitions in recent years [16]. Nevertheless, the corresponding experimental verification proved to be extremely difficult [28]. Eq. (12) provides us a feasible way to measure the fidelity susceptibility in experiments via the neutron scattering or ARPES technique. Therefore, the equality makes the fidelity approach to quantum criticality not merely a theoretical topic. On the other hand, Eq. (12) reveals that the resonance peak in the spectral function denotes a quantum criticality-like point at which the solid state of the sample system seemingly undergoes a significant change. Such an interpretation provides us a new angle to understand the spectral function from the viewpoint of quantum information science.

In Ref. [9], when we defined the concept of dynamic fidelity susceptibility $\chi_F(\eta)$, the variable η was introduced solely for mathematical purpose to due with the Fourier transformation in the complex plane. Since then, no work has ever touched the further meaning of η . In the equality in Eq. (12), we find it is η that connects the two seemingly unrelated quantities from two distinct fields. Moreover, η appends more physical understanding from the equality. From the definition of the fidelity susceptibility, η is the strength of the perturbation. While in the definition of the spectral function, η actually denotes the half-width of the resonance peaks. The uncertainty property of η even relates to the lifetime of the quasi-particle of the resonance peak.

To see the role of the equality in Eq. (12) in quantum phase transitions, in the following, we take the one-dimensional transverse-field Ising model as an example

to show how to measure the fidelity susceptibility in experiments. The model's Hamiltonian reads

$$H = - \sum_{j=1}^N (\sigma_j^z \sigma_{j+1}^z + h \sigma_j^x), \quad (14)$$

where $\sigma_j^{x,y,z}$ is the Pauli Matrix for the 1/2-spin at site j , h is the transverse field, and N is the number of spins. The periodic boundary conditions are assumed. The ground state of the Ising model has two distinct phases, which are the ferromagnetic phase favored by the ferromagnetic Ising interaction in the Hamiltonian and the paramagnetic phase due to the transverse field along $+x$ direction. The competition between them leads to a quantum phase transition occurring at $h_c = 1$.

The one-dimensional quantum Ising model can be realized by several materials. An excellent material is the insulating Ising ferromagnet CoNb_2O_6 whose spin dynamics can be measured by neutron scattering [30]. The model is defined on the zigzag structure formed by Co^{2+} ions whose ferromagnetic coupling is about 1 meV (according to a magnetic field of $10\text{T} \sim 1\text{meV}$). Then the critical field of the systems is about $h = 5.5\text{T}$ which is attainable in the laboratory [30].

Theoretically, the model can be diagonalized by the Jordan-Wigner transformation

$$\sigma_j^z = 1 - 2c_j^\dagger c_j, \quad \sigma_j^+ = \prod_{n < j} \sigma_n^z c_j, \quad (15)$$

the Fourier transformation

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{-ikj} c_k, \quad (16)$$

and the Bogoliubov transformation

$$c_k = u_k b_k + i v_k b_{-k}^\dagger, \quad (17)$$

where c_j is the annihilation operator for spinless fermions at site j . With the diagonalization condition

$$u_k^2 - v_k^2 = \cos 2\theta_k = \frac{-(\cos k - h)}{\sqrt{(\cos k - h)^2 + \sin^2 k}}, \quad (18)$$

$$2u_k v_k = \sin 2\theta_k = \frac{-\sin k}{\sqrt{(\cos k - h)^2 + \sin^2 k}}, \quad (19)$$

the Hamiltonian becomes

$$H = \sum_k \epsilon(k) (2b_k^\dagger b_k - 1), \quad (20)$$

where b_k and b_k^\dagger are fermionic operators, and $\epsilon(k) = \sqrt{1 - 2h \cos(k) + h^2}$ is the dispersion relation of the quasi-particles of b_k^\dagger .

Fidelity approach: From Eq. (20), we see that the ground state of the system is the vacuum state of b_k^\dagger ,

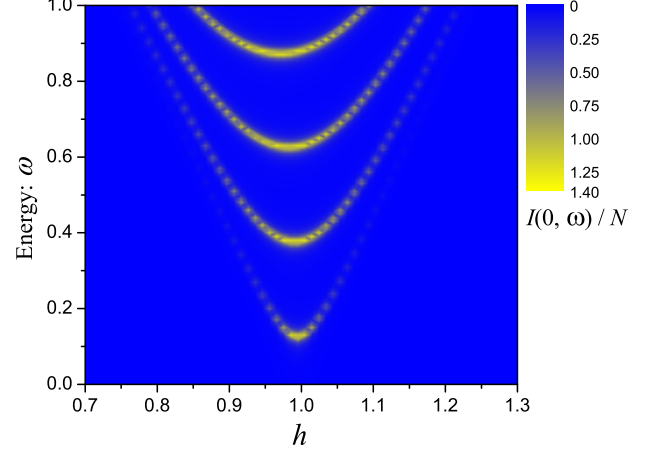


FIG. 1: (Color online) The spectral function $I(k=0, \omega)$ as a function of ω and h . Here $N = 100$ and $\eta = 0.01$.

i.e. $b_k|\psi_0\rangle = 0$. Since $b_k(b_k^\dagger)$ depends on the driving parameter h , to compare the two ground states, we should define them in the space of c_k and c_k^\dagger . The ground state can then be written as

$$|\psi_0\rangle = \prod_{k>0} (\cos \theta_k |0_k, 0_{-k}\rangle + i \sin \theta_k |1_k, 1_{-k}\rangle),$$

where $|1_k\rangle = c_k^\dagger |0_k\rangle$. Under the same basis, the fidelity between two ground states becomes

$$F(h, h') = |\langle \psi_0(h) | \psi_0(h') \rangle| = \prod_{k>0} \cos(\theta_k - \theta'_k).$$

The fidelity susceptibility, as the leading term in the expansion of $F(h, h')$, can be calculated explicitly [3] as

$$\chi_F = \sum_{k>0} \left(\frac{d\theta_k}{dh} \right)^2, \quad (21)$$

where

$$\frac{d\theta_k}{dh} = \frac{1}{2} \frac{\sin k}{1 - 2h \cos k + h^2}. \quad (22)$$

Spectral function: In order to measure the fidelity susceptibility in experiments, we introduce

$$\sigma_k^\pm = \sum_j e^{\mp ijk} \sigma_j^\pm, \quad (23)$$

where $\sigma_j^+ + \sigma_j^- = \sigma_j^x$. Let $A_k = \sigma_k^+ + \sigma_k^-$, then $A_{k=0} = \sum_{j=1}^N \sigma_j^x$ is just the driving term of the Hamiltonian. The spectral function of A_k can be written as

$$I(k, \omega + i\eta) = \sum_n \langle \psi_n | A_k | \psi_0 \rangle^2 \delta(E_0 - E_n + \omega + i\eta). \quad (24)$$

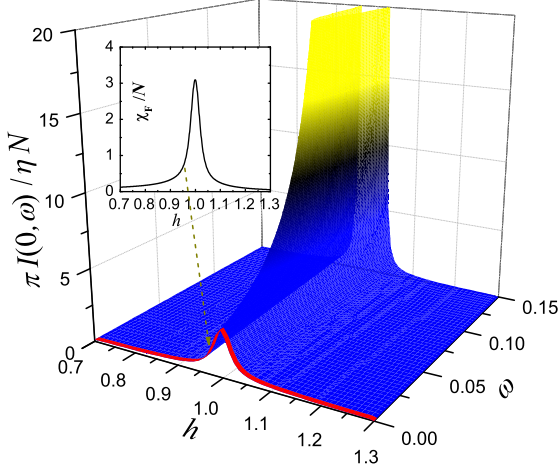


FIG. 2: (Color online) A 3D plot of the re-scaled spectral function as a function of ω and h . The inset is the fidelity susceptibility as a function of h for the Ising model, calculated from Eq. (21). Here $N = 100$ and $\eta = 0.01$. The red line on the 3D surface at $\omega = 0$ is consistent with fidelity susceptibility in the inset, hence $\chi_F \simeq \frac{\pi}{\eta} I(0, i\eta)$ with $\eta = 0.01$.

Let $k = 0$,

$$A_0 = N - 2 \sum_k [(u_k^2 - v_k^2) b_k^\dagger b_k + i u_k v_k (b_k^\dagger b_{-k}^\dagger + b_k b_{-k}) + v_k^2]. \quad (25)$$

Since the ground state is the vacuum state of b_k , the only contribution to the spectral function is the term $4 \sum_{k>0} i u_k v_k b_k^\dagger b_{-k}^\dagger$. We find that the spectral function becomes

$$I(0, \omega + i\eta) = \sum_{k>0} \frac{4 \sin^2 k}{\epsilon(k)^2} \delta[4\epsilon(k) - \omega - i\eta]. \quad (26)$$

In terms of the Poisson kernel representation of the δ -function, we have

$$I(0, \omega + i\eta) = \sum_{k>0} \frac{\eta}{\pi} \frac{4 \sin^2 k}{\epsilon(k)^2} \frac{1}{[4\epsilon(k) - \omega]^2 + \eta^2}. \quad (27)$$

In Fig. 1, we plotted the spectral function as a function of energy ω and the driving parameter h for a system of $N = 100$ and $\eta = 0.01$. According to the color scale definition, the bright region denotes the resonance peaks of the spectral function. We can see that the farther away from the critical point, the higher energy that the first peak locates. This observation is consistent with the structure of the energy spectrum of the quantum Ising

model in which it is gapless only at the critical point. To extract the fidelity susceptibility from the spectral function, we plotted a 3D surface map of the spectral function $I(0, \omega + i\eta)$ as a function of ω and h for the same system and η in Fig. 2. Clearly, though the spectral function becomes smaller and smaller as the energy tends to zero, a line with sharp peak appears in the cross-section of $\omega = 0$. This line is the fidelity susceptibility of the quantum Ising model. As a comparison, we reproduce the fidelity susceptibility of the quantum Ising model in the inset of Fig. 2. These two lines are matched with each other. This fact means

$$\chi_F \simeq \frac{\pi}{\eta} I(0, i\eta) \Big|_{\eta=0.01} \quad (28)$$

for the present system. Therefore, by probing the spectral function of A_k , one can obtain the ground-state fidelity susceptibility which can help us to find the critical point of the system. While Eqs. (12) and (13) are more general in physics, we need $I(0, i\eta)$ only to get the fidelity susceptibility in quantum phase transitions. On the other hand, since A_k in Eq. (24) can be any driving operator of many-body systems, as a more precise form of Eq. (28), the equality

$$\chi_F = \lim_{\eta \rightarrow 0} \frac{\pi}{\eta} I(0, i\eta) \quad (29)$$

is universally valid for any quantum phase transition.

In summary, we derived an interesting equality that relates the fidelity susceptibility and spectral function in this work. Such an equality makes it possible to measure the fidelity susceptibility directly in experiments via the well known techniques, such as neutron scattering, ARPES techniques, etc. Then we investigated the feasibility of probing quantum criticality by measuring the fidelity susceptibility in experiments. For this purpose, we take the one-dimensional transverse-field Ising model as an example because the model can be realized by the compound material CoNb_2O_6 in the laboratory. We show that the fidelity susceptibility can be derived from the spectral function of the driving operator of the model. Due to the important role of the fidelity in detecting quantum phase transitions, we hope that equality will attract experimentalists to study critical phenomena by measuring the fidelity susceptibility directly in experiments.

SJGu thanks Ming Gong for helpful discussions. This work is supported by the Earmarked Grant Research from the Research Grants Council of HKSAR, China, under project CUHK 401212.

[1] S. Sachdev, *Quantum Phase Transitions*, (Cambridge University Press, Cambridge, UK, 2000).

[2] M. A. Nilesen and I. L. Chuang, *Quantum Computation*

- and *Quantum Information* (Cambridge University Press, Cambridge, England, 2000).
- [3] P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123 (2006).
 - [4] H. Q. Zhou and J. P. Barjaktarevic, J. Phys. A: Math. Theor. **41**, 412001 (2008).
 - [5] P. Zanardi, M. Cozzini, and P. Giorda, J. Stat. Mech. **2**, L02002 (2007).
 - [6] M. Cozzini, P. Giorda, and P. Zanardi, Phys. Rev. B, **75**, 014439 (2007).
 - [7] M. Cozzini, R. Ionicioiu, and P. Zanardi, Phys. Rev. B, **76**, 104420 (2007).
 - [8] P. Buonsante and A. Vezzani, Phys. Rev. Lett. **98**, 110601 (2007).
 - [9] W. L. You, Y. W. Li, and S. J. Gu, Phys. Rev. E **76**, 022101 (2007).
 - [10] P. Zanardi, P. Giorda and M. Cozzini, Phys. Rev. Lett. **99**, 100603 (2007).
 - [11] H. Q. Zhou, R. Orus and G. Vidal, Phys. Rev. Lett. **100**, 080601 (2008).
 - [12] Marek M. Rams and Bogdan Damski, Phys. Rev. Lett. **106** 055701 (2011).
 - [13] S. Chen, L. Wang, Y. Hao and Y. Wang, Phys. Rev. A **77**, 032111 (2008).
 - [14] L. C. Venuti and P. Zanardi, Phys. Rev. Lett. **99**, 095701 (2007).
 - [15] S. J. Gu, H. M. Kwok, W. Q. Ning and H. Q. Lin, Phys. Rev. B **77**, 245109 (2008).
 - [16] S. J. Gu, Int. J. Mod. Phys. B **24**, 4371 (2010).
 - [17] A. Hamma, W. Zhang, S. Haas and D. A. Lidar, Phys. Rev. B **77**, 155111 (2008).
 - [18] J. H. Zhao and H. Q. Zhou, Phys. Rev. B **80**, 014403 (2009).
 - [19] S. Yang, S. J. Gu, C. P. Sun and H. Q. Lin, Phys. Rev. A **78**, 012304 (2008).
 - [20] D. F. Abasto, A. Hamma and P. Zanardi, Phys. Rev. A **78**, 010301(R) (2008).
 - [21] T. C. Tzeng, H. H. Hung, Y. C. Chen and M. F. Yang, Phys. Rev. A **77**, 062321 (2008).
 - [22] H. M. Kwok, W. Q. Ning, S. J. Gu and H. Q. Lin, Phys. Rev. E **78**, 032103 (2008).
 - [23] J. Ren, X. Xu, L. Gu, J. Li, Phys. Rev. A **86**, 064301(2012).
 - [24] S. Greschner, A. K. Kolezhuk, and T. Vekua, Phys. Rev. B **88**, 195101 (2013).
 - [25] T. P. Oliveira and P. D. Sacramento, Phys. Rev. B **89**, 094512 (2014); P. D. Sacramento, N. Paunković, and V. R. Vieira, Phys. Rev. A **84**, 062318 (2011).
 - [26] F. Trouselet, P. Horsch, A. Mleé, and W. L. You, Phys. Rev. B **90**, 024404 (2014).
 - [27] X. Luo, K. Zhou, W. Liu, Z. Liang, and Z. Zhang, Phys. Rev. A **89**, 043612 (2014).
 - [28] J. Zhang, X. Peng, N. Rajendran and D. Suter, Phys. Rev. Lett. **100**, 100501 (2008).
 - [29] Riccardo Comin and Andrea Damascelli, *ARPES: A probe of electronic correlations* in the book *Strongly Correlated Systems: Experimental Techniques*, edited by A. Avella and F. Mancini, Springer Series in Solid-State Sciences Vol. 180 (2013).
 - [30] R. Coldea, D. A. Tennant, E. M. Wheeler, E. Wawrzynska, D. Prabhakaran, M. Telling, K. Habicht, P. Smeibidl, K. Kiefer, Science **327**, 177 (2010).